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Momentum transfer and rotational transition cross sections for collision of slow electrons with HCN

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Abstract: The momentum transfer and rotational transition cross sections for collisions of slow electrons with HCN have been calculated in the energy range 0·01 to 0·1 ev by using the Born approximation. For momentum transfer cross section the calculated values are in fairly good agreement with the available experimental data. For the rotational transition cross sections, no such comparison is possible.

1. Introduction

Momentum transfer and rotational transition cross sections by low energy electrons in diatomic, polyatomic gases have been studied by many authors But so far no investigation has been carried out for HCN gas which is a very important constituent of the interstellar medium and has special astrophysical interest (Green and Thaddeus 1974). Here we have calculated both the momentum transfer and rotational transition cross section for electrons in HCN in the energy range 0·01 ev to 0·1 ev, using Born approximation It is found that the agreement between experimental (Tice and Kivelson 1967) and theoretical momentum transfer cross section data is good, but due to non availability of experimental data such comparison for rotational transition cross section is not possible The interaction potential for *e*-HCN collisions has been carefully constructed taking into account both short and long range forces

2. Formulation

The potential energy of interaction between an electron and a molecule is given by

$$V(\mathbf{r}, \hat{\mathbf{s}}) = \sum_{\lambda=0} V_\lambda P_\lambda (\hat{\mathbf{r}}, \hat{\mathbf{s}})$$

$$- V^{SR}_{HCN} + V^{\mu}_{HCN} + V^{\textcircled{S}}_{HCN} + \cdots$$

$$- v_H(r_H) + v_C(r_C) + v_N(r_N) - \frac{e\mu}{r^2} P_1(\hat{\mathbf{r}}, \hat{\mathbf{s}}) - \left(\frac{e\textcircled{S}}{r^3} + \frac{e^2\alpha'}{r^4} \right) P_2(\hat{\mathbf{r}}, \hat{\mathbf{s}}) + \cdots \quad (1)$$

The symbols used here have their usual physical significances. The short range electrostatic potential of HCN is the sum of the electrostatic potentials of H, C and N atoms, given by

$$V_{HCN}^{SR} = v_H(r_H) + v_C(r_C) + v_N(r_N)$$

The short range potential used for hydrogen is derived from the relation (Geltman and Takayanagi 1966)

$$v_H(r_H) = -A_H \exp[-a_H |r_H - S/2|] \tag{2}$$

S, is the internuclear distance

For simplicity of calculation this is fitted to the form

$$v_H(r_H) = -\frac{A_H}{r_H} \exp[-a_H r_H] \tag{3}$$

where $A_H = 25{\cdot}25\ a_0$, $a_H = 3{\cdot}13\ a_0^{-1}$.

The short range interactions e-C and e-N have been estimated by following the method of Ray and Barua (1974).

Using Born approximation the differential scattering cross section for the transition $\Delta j = \pm 1$ is given by

$$\frac{d\sigma'}{d\Omega}(j \to j') = \frac{4}{3} \frac{m}{K^2} \frac{k'}{k} (\mu + I_1 + I_2 + \ldots + I_6)^2 C^2(j1j', 000) \tag{4}$$

where $\hbar K$ is the change in relative momentum, m is the reduced mass, k and k' are the wave numbers corresponding to states j and j' respectively, C is the Clebsch-Gordan coefficient and I's are integrals of which I_1 is given by

$$I_1 = M \left[\int_0^{R_H} e^{a_H r} \left(1 - \frac{1}{a_H r}\right) + e^{-a_H r} \left(1 + \frac{1}{a_H r}\right) \right] \left(\frac{\sin(Kr)}{Kr} - \cos(Kr) \right) dr \tag{5}$$

Similar expressions may be obtained for the other integrals in equation (4).

For the transition $\Delta j = 0, \pm 2$, the differential cross section is given by

$$\frac{d\sigma'}{d\Omega}(j \to j'')$$

$$= \frac{4m}{5} \frac{k''}{k} \left[\left(\frac{\Theta}{3} + \frac{e\alpha' \pi K}{16} \right) + \frac{1}{K} (I'_1 + I'_2 + \ldots + I'_6) \right]^2 C^2(j2j'', 000) \tag{6}$$

I's are integrals of which I'_1 is given by

$$I'_1 = N \int_0^{R_H} \left[e^{a_H r} \left(1 - \frac{3}{a_H r} + \frac{3}{a_H^2 r^2} \right) - e^{-a_H r} \left(1 + \frac{3}{a_H r} + \frac{3}{a_H^2 r^2} \right) \right]$$

$$\left[\left(\frac{3}{k^2 r^2} - 1 \right) \sin(Kr) - \frac{3}{kr} \cos(Kr) \right] dr. \qquad (7)$$

Similar expressions may be obtained for the other integrals in equation (6). In equations (5) and (7) the two constants M and N are given by

$$M = \frac{3A_H e^{-a_H r}}{2a_H r} - \left(1 + \frac{1}{a_H r} \right)$$

$$N = \frac{5A_H e^{-a_H r}}{2a_H r} \left(1 + \frac{3}{a_H r} + \frac{3}{a_H^2 r^2} \right)$$

The integral cross section for the transition j to l is given by,

$$\sigma'(j \to l) = \frac{2\pi}{kq} \int_{k-q}^{k+q} \frac{d\sigma'}{d\Omega} \, KdK \qquad (8)$$

Putting the values of $d\sigma'/d\Omega$ from equation (4) and equation (6) in equation (8) we get the integral cross sections for different transitions $j \to j \pm 1$ and $j \to j \pm 2$.

The momentum transfer cross section for the transition $j \to l$ is defined as,

$$\sigma_m(j \to l) = \int (1 - \hat{k}\,\hat{q}) d\sigma(j \to l) \qquad (9)$$

Substituting the value of $d\sigma$ from equations (4) and (6) we can calculate the momentum transfer cross section from equation (9)

3. Results and discussion

For HCN we have considered only the transitions from the ground rotational state, the cross sections $\sigma(0 \to 0)$, $\sigma(0 \to 1)$, $\sigma(0 \to 2)$ are obtained in the energy range 0·01 ev to 0·1 ev. The dipole and quadrupole moments are taken as 1·175 ea_0 and 3·27 ea_0^2 respectively (Stogryn and Stogryn 1966) and polarizability as 4·454 a_0^3 (Hirschfelder *et al* 1966).

The integral cross section for different transitions is calculated from equation (8) and plotted in Figure 2 The momentum transfer cross section is also calculated from equation (9) for the energy range 0·01 ev to 0·1 ev and plotted in Figure 1

We find from the figures that both the momentum transfer and rotational transition cross section values increase when we take account of the short range effect. This difference also increases with the increase of energy 2% to 20%. The agreement between experimental (Tice and Kivelson 1967) and theoretical momentum transfer cross section data considering short range effect is good.

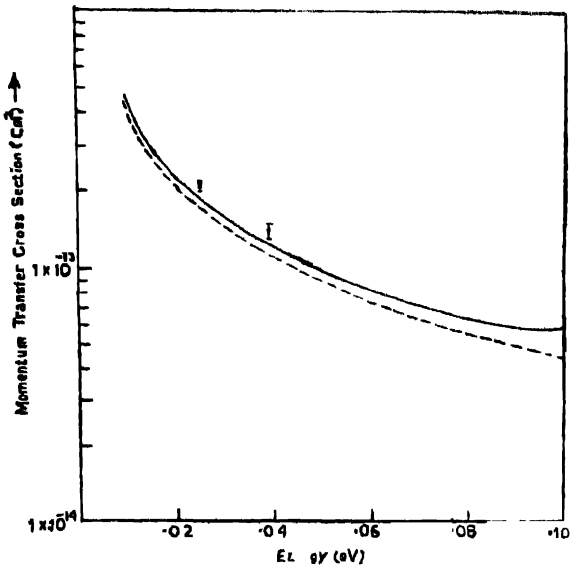

Figure 1. Momentum transfer cross section for electrons in HCN gas; solid curve considering short range forces; - - - - without short range, q· experimental

Due to non availability of experimental data in the case of rotational transition such comparison between theory and experiment is not possible.

Itikawa and Takayanagi (1969) compared the Born results with the close coupling calculations for rotational transition cross sections in electron polar molecular collisions. They found that at low energies ($\sim 0{\cdot}1$ ev) even for molecules having sizeable dipole moment ($\sim$ 1 a.u) the maximum difference between the Born and close coupling calculations is 20%. Thus for HCN which has a dipole moment of 1·1 a u. similar limit of maximum error due to our use of the Born approximation is expected For close encounters due to the increase in the strength of interaction the Born approximation will yield much larger cross sections than those given by close coupling calculations (Itikawa and Takayanagi 1969). However its effect on the integral cross section will be much less as stated above.

Another source of error in our calculations is the inaccuracy in our estimation of the short range interaction The main factor is the addition of the individual electron atom collision terms which overestimates the interaction. However at low energies the error thus introduced is expected to be much less than that introduced by the Born approximation.

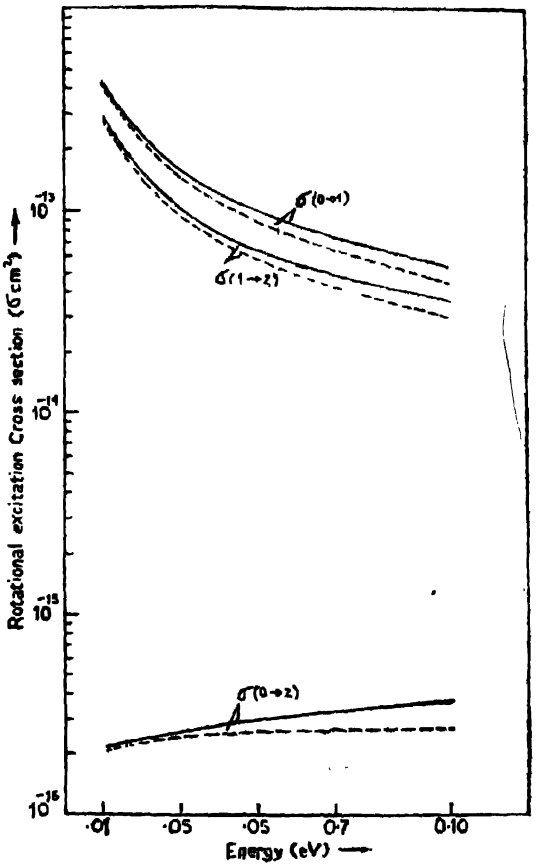

Figure 2. Rotational transition cross section for electron in HCN gas; solid curve considering short range forces; - - - - without short range.

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